HRTEM Image Simulation of Fine Particles

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The technique of high-resolution transmission electron microscopy (HRTEM) has proven to be very useful for characterization of nanocrystalline particles, particularly for catalysts (for useful reviews see Malm et al.[1-3]). As in the case of large crystals, interpretation of HRTEM images of nanocrystals requires some care. For large crystalline areas, the standard method of image interpretation in terms of specimen structure is by comparison of experimental images with simulated crystal-structure images computed under the appropriate electron microscope conditions.[4] Although such image simulations are routinely carried out for "semi-infinite" models of crystalline specimens, they can also be used to produce useful information from particle images, such as the crystal structures of the particles, as well as their approximate shapes, sizes, and orientations.[5] However, for accurate simulations of nanocrystal images, the calculation must be modified to allow the specimen model to contain the crystal edges. Early simulations of HRTEM images of edges[6,7] showed that the supercell method of model construction, previously developed for embedded defects[8], also works for these cases. Simulations of complete models of nanoparticles are now routinely used to interpret experimental particle images.[9-12]

Systematic investigations into HRTEM images of nanoparticles using image simulations have shown that the appearance of the particles -- particularly their shapes[11] and internal structures[12] -- is critically dependent on the electron microscope imaging conditions. Simulations show that Fresnel fringes can lead to the illusion of "relaxations" of the outer atom rows, and even to the appearance of rows of "ghost" atoms in the HRTEM image, far outside the outermost layer of atoms; such effects can produce distorted measurements of the sizes (overestimates of up to 25%) and shapes of the nanocrystals.[11]

Fields of randomly-oriented nanocrystalline catalyst particles typically produce HRTEM images that show fringes within most of the nanocrystals. HRTEM image simulations confirm that most orientations of model nanocrystals will produce fringes; these fringes, although deceptively like lattice fringes, are *not* simply related to the crystal structure of the particle. In general, "lattice spacings" measured from fringes appearing in randomly-oriented particles will be in error. In addition, depending strongly upon the orientation of the particle, images of a perfect nanocrystal can show details that are easily misinterpretable as "relaxations", "bent planes", and even "twinned" areas.[3,12]

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